METHODS FOR DETERMINING POLYPEPTIDE STRUCTURE, FUNCTION OR PHARMACOPHORE FROM COMPARISON OF POLYPEPTIDE SEQUENCES

ABSTRACT OF THE DISCLOSURE

The invention provides a method for separating 5 two or more subsets of polypeptides within a set of The method includes the steps of: polypeptides. determining a sequence comparison signature for each amino acid sequence in a set of amino acid sequences, wherein the sequence comparison signature includes 10 pairwise comparison scores for the amino acid sequence compared to each of the other amino acid sequences in the (b) constructing a distance arrangement including the sequence comparison signatures related according to the distance between each of the sequence comparison 15 signatures; and (c) identifying a first and second cluster of sequence comparison signatures in the distance arrangement, wherein the first cluster includes sequence comparison signatures for polypeptides having a similar protein fold or biological function, the protein fold or 20 function being different compared to a protein fold or function of polypeptides having sequence comparison signatures in the second cluster.